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Modeling High-Pressure and High-Temperature Behavior of Chemically Reactive Systems

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Abstract

Some of interesting changes that occur in nature contain mixtures at high pressure (up to tens of giga Pascal) and high temperatures (at several thousand Kelvins). They may involve phase changes and chemical reactions with many chemical species. This field of physics and chemistry is relevant to high explosives and, hence, has been richly supported by experimental data but poorly explored by theoreticians. Fortunately, for simple systems or complex molecular mixtures at high temperatures, it is possible to develop a reliable statistical mechanical model based on molecular physics, an accurate theory of fluids, and the thermodynamic equations governing multiphase chemical equilibria.

We will describe such a mixture model and apply them to experimental high explosives data. Results predict (1) a possibility of fluid-fluid phase separations; (2) information on unlike-pair intermolecular potentials of various chemical species, and (3) slow condensation process of carbon clusters. This paper will describe each of these aspects in details and a nonequilibrium model involving carbon coagulation on high explosives properties.

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